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NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB

NEWS 43 Jun 06 PASCAL enhanced with additional data

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FILE COVERS 1907 - 14 Jun 2003 VOL 138 ISS 25 FILE LAST UPDATED: 13 Jun 2003 (20030613/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s JP 5365865/pn

0 JP 5365865/PN (JP5365865/PN) => s JP 65865/pn0 JP 65865/PN (JP65865/PN) => s JP 51-140578/pn0 JP 51-140578/PN L3 (JP51140578/PN) => s gb 1570597/pn 1 GB 1570597/PN (GB1570597/PN) => d l4 ibib hitstr L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1977:584771 CAPLUS 87:184771 DOCUMENT NUMBER: 16.beta.-Alkylestradiol derivatives TITLE: Miki, Takuichi; Hiraga, Kentaro; Goto, Giichi INVENTOR(S): Takeda Chemical Industries, Ltd., Japan PATENT ASSIGNEE(S): SOURCE: Ger. Offen., 24 pp. CODEN: GWXXBX DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: KIND DATE PATENT NO. APPLICATION NO. DATE ______ ----_____ DE 2653558 A1 19770608 DE 1976-2653558 19761125 JP 52065259 A2 19770530 JP 1975-142509 19751127 JP 61044878 B4 19861004 GB 1570597 GB 1976-49180 A 19800702 19761125 <--A1 19770624 FR 1976-35824 FR 2332999 19761126 B1 19790406 FR 2332999 CA 1076102 A1 19800422 CA 1976-266709 19761126 CH 629221 A 19820415 CH 1976-14943 19761126 PRIORITY APPLN. INFO.: JP 1975-142509 19751127 => s 16beta-ethylestradiol 4 16BETA 42 ETHYLESTRADIOL 0 16BETA-ETHYLESTRADIOL L5 (16BETA (W) ETHYLESTRADIOL) => s 16 beta-ethylestradiol 700644 16 1194130 BETA 42 ETHYLESTRADIOL 7 16 BETA-ETHYLESTRADIOL

(16(W) BETA(W) ETHYLESTRADIOL)

=> s 16 beta-n-butylestradiol

700644 16
1194130 BETA
2585772 N

1 BUTYLESTRADIOL

L7 0 16 BETA-N-BUTYLESTRADIOL
(16(W) BETA(W) N (W) BUTYLESTRADIOL)

=> s 16 beta-butylestradiol
700644 16
1194130 BETA
1 BUTYLESTRADIOL

L8 0 16 BETA-BUTYLESTRADIOL
(16(W) BETA(W) BUTYLESTRADIOL)

=> s butylestradiol

L9 1 BUTYLESTRADIOL

=> d 19 ibib hitstr abs

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1957:51924 CAPLUS

DOCUMENT NUMBER: 51:51924

ORIGINAL REFERENCE NO.: 51:9659i,9660a-i,9661a

TITLE: 17-Alkyl-19-nortestosterones

AUTHOR(S): Colton, Frank B.; Nysted, Leonard N.; Riegel, Byron;

Raymond, Albert L.

CORPORATE SOURCE: G. D. Searle & Co., Chicago

SOURCE: J. Am. Chem. Soc. (1957), 79, 1123-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

17-Ethynyl-19-nortestosterone (8.6 g.) in 350 cc. dry dioxane hydrogenated over 1.1 g. 5% Pd-C until 2 moles H were absorbed, filtered, and evapd. to dryness in vacuo, and the residue chromatographed with 20-30% EtOAc in C6H6 on 450 g. silica gel yielded 6.12 g. 17-ethyl-19-nortestosterone (I), m. 137-8.degree. (from aq. MeOH), [.alpha.]D 25.degree. (c 1, CHCl3). A slow stream of C2H2 passed over the surface of a stirred soln. of 5.0 g. K in 100 cc. Me3COH and 100 cc. dry Et2O at 0.degree. until satd., treated with 5.0 g. Me estrone, the addn. of C2H2 continued 3-4 hrs. at 0.degree., the mixt. kept 18 hrs. at room temp., treated with 100 cc. 10% aq. NH4Cl, steam distd., and filtered, and the residue crystd. from Me2CO gave 5.1 g. 17-ethynylestradiol 3-Me ether (II), m. 150-1.5.degree.. II (5.0 g.) in 75 cc. purified dioxane hydrogenated over 0.5 g. 5% Pd-C until 2 moles H was absorbed, filtered, and evapd. to dryness in vacuo yielded 4.8 g. 17-ethylestradiol 3-Me ether (III), m. 85-7.degree. (from Me2CO-petr. ether). III (4.0 g.) in 100 cc. dry Et20 and 300 cc. liquid NH3 stirred 1 hr. with 4.0 g. Li, treated dropwise during 1.5 hrs. with 30 g. EtOH dild. with an equal vol. of dry Et20 while using an addnl. 100 cc. dry Et20 to wash the sides of the flask during the EtOH addn., the NH3 evapd. with gentle warming, the mixt. dild. with 100 cc. cold H2O, and the product isolated by extn. gave 3.4 g. 17-ethyl-1,4-dihydroestradiol 3-Me ether (IV), m. 126-8.degree. (from Et20-MeOH). IV (1.25 g.) in 20 cc. MeOH refluxed 5 min. with 2.2 cc. glacial AcOH and dild. with 100 cc. H2O gave 1.15 g. 17.alpha.-ethyl-17-hydroxy-5(10)-estren-3-one, m. 134-6.degree. (from Me2CO-petr. ether). IV (2.0 g.) added with stirring to 2.4 cc. concd. HCl and 1.6 cc. H2O in 36 cc. MeOH, allowed to stand 2 hrs. at room temp., and filtered gave 1.7 g. I, m. 136-9.degree. (from Me2CO-petr.

17-Octynylestradiol 3-Me ether (3.0 g.) in 75 cc. purified dioxane hydrogenated over 0.5 g. 5% Pd-C until 2 moles H was absorbed, filtered, and evapd., and the residue triturated with MeOH gave 1.9 g. 17-octylestradiol 3-Me ether (V), m. 79-81.degree., [.alpha.]D 40.degree. (c 1.25, CHCl3). V (1.5 g.) subjected to a Birch reduction gave 1.2 g. solvated cryst. material which became amorphous on drying in vacuo; the amorphous material cleaved and isomerized in the usual manner yielded 0.8 g. 17-octyl-19-nortestosterone, m. 120-2.degree. (from aq. MeOH). II (4.0 g.) reduced in the usual manner yielded 3.1 g. 3-methoxy-19-norpregna-2,5(10),17-(20)-triene (VI), m. 111-12.degree.. VI (1.0 g.) isomerized in the usual manner with HCl gave 0.76 g. 19-norpregna-4,17-(20)-dien-3-one, m. 124-5.degree.. Mg (8.5 g.) (activated with iodine) covered with 200 cc. dry Et20, treated dropwise with 5.0 g. CH2: CHCH2Br in 20 cc. dry Et20, and then during 45 min. with 20.0 g. estrone Me ether in 95 g. CH2:CHCH2Br and 400 cc. Et2O, refluxed 2.5 hrs., cooled, and treated with 500 cc. 10% aq. NH4Cl, and the Et2O layer worked up yielded 18.4 g. 17-allylestradiol 3-Me ether (VII), m. 91-1.5.degree. (from Et20-petr. ether), [.alpha.]D 57.4.degree. (c 1.02, CHCl3). VII (11.5 g.) in 200 cc. EtOH hydrogenated over 5 g. 5% Pd-C until 1 mole H had been absorbed, filtered, and evapd. in vacuo yielded 10.1 g. 17-propylestradiol 3-Me ether (VIII), m. 93-4.degree. (from Et20-MeOH], [.alpha.]D 47.7.degree.. VIII (6.0 g.) reduced with Li in NH3 gave 4.7 g. 17-propyl-1,4dihydroestradiol 3-Me ether (IX), m. 150-2.degree., [.alpha.]D 105.degree. (c 1.16, CHCl3). VII (5.0 g.) hydrogenated in dioxane over 5% Pd-C yielded 4.0 g. IX, m. 149-51.degree.. IX (1.0 g.) in MeOH heated with glacial AcOH gave 0.8 g. 17.alpha.-propyl-17-hydroxy-5(10)-estren-3-one, m. 90.0-1.5.degree.. IX (1.8 g.) cleaved and isomerized in the usual manner yielded 1.4 g. 17-propyl-19-nortestosterone, m. 122-3.degree., [.alpha.]D 21.degree. (c 0.98, CHCl3). 1,4-Dihydroestradiol 3-Me ether (25 g.) in 242 cc. cyclohexane and 860 cc. PhMe refluxed 2 hrs. with 25 g. (iso-PrO)3Al in 347 cc. PhMe, treated dropwise during 10 min. with 169 cc. satd. aq. Rochelle salt, and steam distd., the aq. distn. residue filtered, and the solid product triturated with 100 cc. MeOH and cooled to O.degree. gave 21.0 g. 1,4-dihydroestrone 3-Me ether (X), m. 141-1.5.degree. (from MeOH). Mg (1.7 g.) (activated with iodine) treated with 9.0 g. CH2: CHCH2Br in 100 cc. Et2O, refluxed 15 min., treated with 2.0 g. X in 100 cc. Et2O, refluxed 1.5 hrs., and treated slowly with 100 cc. 10% aq. Rochelle salt, the Et20 layer worked up, the residue dissolved in 40 cc. MeOH, 1.5 cc. concd. HCl, and 5 cc. H2O, kept 2 hrs. at room temp., and dild. with 200 cc. cold H2O, and the crude ppt. chromatographed on 150 g silica gel yielded 1.1 g. 17-allyl-19-nortestosterone, m. 93-5.degree.. 1-Octyne (24 g.) in 125 cc. dry Et20 stirred 1 hr. at O.degree. with 7.8 g. EtMe2COK (from 7.8 g. K), treated with 5.7 g. estrone Me ether, warmed to room temp., stirred 24 hrs., and treated with 150 cc. 10% NH4Cl, the org. layer worked up, and the residue chromatographed with 0.5% C6H6 in CHCl3 on silica gel gave 4.6 g. 17-octynylestradiol Me ether, oil. BuLi (from 9.0 cc. BuBr and 0.67 g. Li) added with stirring to 1.65 g. estrone Me ether in 40 cc. dry Et20, stirred 1 hr., decompd. with MeOH and dil. H2SO4, and dild. with Et2O, the Et20 layer worked up, and the residue chromatographed with 20% Skellysolve A in C6H6 on 100 g. Al2O3 gave 426 mg. 17-butylestradiol 3-Me ether (XI), m. 52-5.degree. partially solidified and remelted at 92-4.degree.. XI subjected to a Birch reduction, cleaved and rearranged, and the crude product chromatographed with 20% EtOAc in C6H6 on 35 g. silica gel yielded 118 mg. 17-butyl-19-nortestosterone, m. 126-7.degree. (from aq. MeOH).

=>

=> d 16 1-7 ibib hitstr abs

L6 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1995:417462 CAPLUS

DOCUMENT NUMBER: 122:170182

TITLE: Therapeutics for treatment of osteoporosis

INVENTOR(S): Miki, Shuji; Kanehira, Koichi; Matsumoto, Toshio

PATENT ASSIGNEE(S): Kuraray Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp. CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 06312930 A2 19941108 JP 1993-128036 19930430

PRIORITY APPLN. INFO: JP 1993-128036 19930430

AB The title therapeutic compns. (e.g. tablets) contain progestogens and estrogen antagonists as active ingredients. Administration of progesterone (I) and 16.beta.-ethylestradilol (II) at 25 mg/kg and 50 .mu.g/kg, resp., s.c. for 2 wk to bone morphogenetic protein-treated rats resulted in bone mineral increase by 60%, vs. -6% or 14%, resp. for I or II alone.

L6 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1992:598537 CAPLUS

DOCUMENT NUMBER: 117:198537

TITLE: Bone resorption inhibitors containing estradiols

INVENTOR(S): Miki, Takuichi; Kumazuki, Takamaru; Yamazaki, Iwao;

Goto, Giichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 04145024 A2 19920519 JP 1990-268575 19901005

PRIORITY APPLN. INFO.: JP 1990-268575 19901005

OTHER SOURCE(S): MARPAT 117:198537

GI

AB Bone resorption inhibitors, which are useful for treatment of osteoporosis and less assocd. with adverse effects, contain estradiols I (R1 = H, alkyl, acyl; R2 = H, alkyl, alkynyl; R3 = alkyl, alkenyl, alkynyl, cyclic hydrocarbyl; R4 = H, cardrocarbyl; the dot line attached to R3 may be bond), their salts, or esters. 16.beta.—

Ethylestradiol (II) at 10 .mu.g/mL inhibited 74.7% resorption of Ca by rat embryo bone, vs. 81.0%, for estradiol. Administration of II at 20 .mu.g/kg to oophorectomized rats did not affect wt. of uterus, vs. severe wt. increase, when estradiol at 0.2 .mu.g/kg was administered instead. Tablets were formulated contg. II 5, lactose 25, starch 98, CMC Ca 20, and Mg stearate 2 g. Several I were prepd.

L6 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1991:527546 CAPLUS

DOCUMENT NUMBER:

DOCUMENT NUMBE

TITLE:

115:127546

Glucocorticoids suppress and estrogens enhance the lipopolysaccharide-induced increase in putrescine and

N1-acetylspermidine in mouse liver

AUTHOR(S):

Sugimoto, Hiroyuki; Hamana, Koei; Matsuzaki, Shigeru;

Arai, Takayuki; Yamada, Shoji

CORPORATE SOURCE:

SOURCE:

Inst. Endocrinol., Gunma Univ., Maebashi, 371, Japan Journal of Steroid Biochemistry and Molecular Biology

(1991), 38(6), 781-6

CODEN: JSBBEZ; ISSN: 0960-0760

DOCUMENT TYPE:

LANGUAGE:

Journal English

AB Administration of lipopolysaccharide (LPS) to mice increases hepatic levels of putrescine (PUT) and N1-acetylspermidine (N1-acetyl-SPD). The in vivo effects of steroid hormones on the LPS-induced increase in PUT and N1-acetyl-SPD were studied in mice. Corticosterone, hydrocortisone, and dexamethasone suppressed the LPS-induced increase in PUT and N1-acetyl-SPD in the liver in a dose-dependent manner, dexamethasone being the most effect among them. Estrone and estradiol-17.beta. enhanced the LPS-induced increase in PUT and N1-acetyl-SPD in a dose-dependent manner. Estradiol-17.alpha. and 16.beta.-ethyl-estradiol, an inactive estradiol isomer and an antiestrogen, resp., enhanced the increase in PUT and N1-acetyl-SPD concns. induced by LPS. Estriol 16.alpha.-hydroxyesterone, 2-hydroxyestradiol, 2-hydroxyesterone, progesterone, testosterone, diethylstilbestrol, and nonsteroidal antiestrogens such as tamoxifen and nafoxidine had no effect on the increase. Estradiol-17.beta. enhanced and corticosterone had little effect on the carbon tetrachloride-induced increase in PUT and N1-acetyl-SPD. Glucocorticoids may suppress the increase by preventing the immunol. injury by Kupffer cells on hepatocytes. The stimulatory effect of estrogens may not be assocd. with their estrogenic activities mediated by the estrogen receptor system.

09779331

ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1979:572408 CAPLUS

DOCUMENT NUMBER:

91:172408

TITLE:

Influence of intrahypothalamic implants of

antiestrogen or aromatase inhibitor on development of sterility following neonatal androgenization in female

rats

AUTHOR(S):

Hayashi, Shinji

CORPORATE SOURCE:

Endocrinol. Div., Natl. Cancer Cent. Res. Inst.,

Tokyo, 104, Japan

SOURCE:

Journal of Steroid Biochemistry (1979), 11(1B), 537-41

CODEN: JSTBBK; ISSN: 0022-4731

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Paraffin micropellets contg. 16.beta.-

ethylestradiol (EED), an antiestrogen or 1,4,6-androstatriene-3,17dione (ATD), an aromatase inhibitor, implanted directly into the hypothalamus of neonatal female rats 6 h prior to a single s.c. injection of testosterone propionate (TP). The antagonists did not impair the sterilizing action of TP but enhanced the induction of sterility. In contrast, intrahypothalamic implantation of paraffin micropellets contg. 1% TP together with 50% MER-25, an antiestrogen, brought about a suppression of sterility induction. The reasons why intrahypothalamic implants of antiestrogen or aromatase inhibitor failed to suppress the sterilizing effect of TP s.c. injected are discussed.

ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1978:597804 CAPLUS

DOCUMENT NUMBER:

89:197804

TITLE:

Estradiol derivatives

INVENTOR(S):

Miki, Takakazu; Hiraga, Kentaro; Goto, Yoshikazu

PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
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JP 53065865		19780612		JP 1976-140578	19761123
PRIORITY APPLN. INFO.	:		JΡ	1976-140578	19761123
GI					

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AB Fourteen estradiol derivs. I (R = alkyl; R1 = H, acyl) were prepd. by ether cleavage or deacylation of II (R2 = alkyl, acyl). I had antiestrogen activity (no data). Thus, a mixt. of 1 g 16. beta -ethylestradiol 3-Me ether and 1.3 g pyridinium chloride was heated 2 h at 150.degree. to give 16.beta -ethylestradiol.

L6 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1978:437039 CAPLUS

DOCUMENT NUMBER:

89:37039

TITLE:

The competitive action of 16.beta

.-ethylestradiol on the binding of estrogen

receptor in human breast cancer

AUTHOR(S):

Takikawa, H.

CORPORATE SOURCE:

Inst. Endocrinol., Gunma Univ., Maebashi, Japan

SOURCE:

Research on Steroids (1977), 7, 291-9 CODEN: RSTEBF; ISSN: 0370-7466

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The cytosol receptor for estrogen was isolated and purified from human mammary gland samples. Most of the 16-substituted estradiols had no effect on binding of 17.beta.-estradiol [50-28-2] but 16.

beta.-ethylestradiol [62633-99-2] inhibited binding strongly. Synthetic estrogens inhibited the binding as did synthetic

antiestrogens. From the compds. tested, the binding affinity was diminished if a phenolic hydroxyl group on C 3 or an alc. hydroxyl group on C 17 was substituted; if both groups were substituted the activity was abolished.

L6 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1977:584771 CAPLUS

DOCUMENT NUMBER:

87:184771

TITLE:

16.beta.-Alkylestradiol derivatives

INVENTOR(S):

Miki, Takuichi; Hiraga, Kentaro; Goto, Giichi

PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan

SOURCE:

Ger. Offen., 24 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2653558	A1	19770608	DE 1976-2653558	19761125
JP 52065259	A2	19770530	JP 1975-142509	19751127
JP 61044878	B4	19861004		
GB 1570597	Α	19800702	GB 1976-49180	19761125
FR 2332999	A1	19770624	FR 1976-35824	19761126
FR 2332999	В1	19790406		
CA 1076102	A1	19800422	CA 1976-266709	19761126
CH 629221	Α	19820415	CH 1976-14943	19761126
PRIORITY APPLN. INFO.	:		JP 1975-142509	19751127
GI				

AB Eight antiestrogenic 16.beta.-alkylestradiols I (R = Et, Me2CH, allyl, Bu, 3-butenyl; Rl = H, Ac, EtCO, PhCH2CH2CO, Bz) were prepd. routinely. Thus, 16.beta.-ethylestradiol 3-Me ether was heated with pyridine at 150.degree. to give I (R = Et, Rl = H), which was acetylated to the diacetate and then selectively hydrolyzed with K2CO3 in MeOH to I (R = Et, Rl = Ac).

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L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 62633-99-2 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-, (16.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 16.beta.-Ethylestra-3,17.beta.-diol

CN 16.beta.-Ethylestradiol

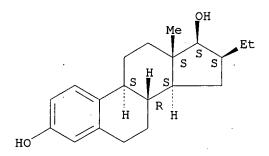
FS STEREOSEARCH

MF C20 H28 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, MEDLINE, USPATFULL

(*File contains numerically searchable property data)

Absolute stereochemistry.



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L1 0 S JP 5365865/PN
L2 0 S JP 65865/PN
L3 0 S JP 51-140578/PN
L4 1 S GB 1570597/PN
L5 0 S 16BETA-ETHYLESTRADIOL
L6 7 S 16 BETA-ETHYLESTRADIOL
L7 0 S 16 BETA-N-BUTYLESTRADIOL
L8 0 S 16 BETA-BUTYLESTRADIOL
L9 1 S BUTYLESTRADIOL
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